International Workshop on

NANOCOMPOSITES: MATERIALS, NEUTRONS AND DATA INTERPRETATION

March 28-30, 2002

Argonne National Laboratory, Argonne, IL, USA

WORKSHOP SCHEDULE

SPEAKER ABSTRACTS

POSTER ABSTRACTS

LIST OF ATTENDEES

Sponsored by Argonne National Laboratory
and the Intense Pulsed Neutron Source

International Workshop on

NANOCOMPOSITES: MATERIALS, NEUTRONS AND DATA INTERPRETATION

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WORKSHOP SCHEDULE

Thursday, March 28, 2002

8:00 – 8:45 REGISTRATION IN BUILDING 362 LOBBY

8:45 – 8:55 WELCOME - **Beverly Hartline**, Deputy Laboratory Director, ANL

8:55 – 9:00 OPENING REMARKS - **Raymond Teller**, Division Director, ANL-IPNS

SESSION I. OVERVIEW – CHAIR: **David Price**, ANL-MSD
9:00 – 9:30 Self Assembly and Nanomaterials
Samuel I. Stupp, Northwestern University
9:30 – 10:00 Application of Neutron Scattering in Nanotechnology
P. Thiyagarajan, ANL-IPNS
10:00 – 10:30 The Spallation Neutron Source: A Powerful Tool for Nanomaterials Research
Thom Mason, ORNL-SNS

10:30 – 10:50 MORNING BREAK

SESSION II. MATERIALS OVERVIEW – CHAIR: **Lennox Iton**, ANL-MSD
10:50 – 11:20 Nanomaterials and Nanotechnology
Richard Siegel, Rensselaer Polytechnic Institute
11:20 – 11:50 From Nanostructured Electroactive Assembly to Molecular p-n Junction
Luping Yu, University of Chicago

11:50 – 1:00 LUNCH IN ROOM F108

SESSION III. MAGNETIC SYSTEMS 1 – CHAIR: **Frank Klose**, ORNL-SNS
1:00 – 1:30 Nano Science and Nano Technology at Argonne
Axel Hoffmann, ANL-MSD
1:30 – 2:00 Probing Magnetic Nanostructures by Neutron Scattering
Suzanne te Velthuis, ANL-MSD
2:00 – 2:30 "Smart" and "Active" Magnetic and Metal-Insulator-Transition Nanocomposite Layers Formed by Ion Implantation
Lynn Boatner, ORNL

2:30 – 2: 50 AFTERNOON BREAK

SESSION IV. MATERIALS & SIMULATIONS 1 – CHAIR: **Gian Felcher**, ANL-MSD
2:50 – 3:20 Ferromagnetic Semiconductors and their Nanostructures: New Opportunities and Challenges
Jacek Furdyna, University Notre Dame
3:20 –3:50 Theoretical Interpretation of Polarized Neutron Reflection and Off-Specular Scattering from Nanocomposite Films
Boris Toperverg, IFF, Julich

SESSION V. POSTERS AND SHORT PRESENTATIONS – CHAIR: **Jyotsana Lal**, ANL-IPNS
3:50 – 4:30 Short Presentations (**Alok Chatterjee, Rex Gerald, Alexander Kolesnikov, Suresh Narayanan, Susana Trasobares-Llorente and Jean-Marc Zanotti**)

4:30 – 6:00 POSTER SESSION IN BUILDING 362 AUDITORIUM LOBBY

6:30 – 9:00 BANQUET AT ARGONNE GUEST HOUSE

Friday, March 29, 2002

8:30 – 9:00	REGISTRATION

SESSION VI. BIOLOGY – CHAIR: **Marion Thurnauer**, ANL-CHM

9:00 – 9:30	Amyloid Structure: Models and Theoretical Considerations for the Construction of Fibrous Nanoscale Self-Assemblies **David Lynn**, Emory University
9:30 – 10:00	Self-Assembled Phases of Biopolymers, Membranes, Proteins, and Counterions **Gerard Wong**, UIUC
10:00 – 10:30	Supermolecular Chain Reaction **Hicham Fenniri**, Purdue University
10:30 – 10:50	MORNING BREAK

SESSION VII. MATERIALS 1 – CHAIR: **Randall Winans**, ANL-CHM

10:50 – 11:20	Nanostructured Materials Based on Block Copolymer Thin Films **Thomas Russell**, University of Massachusetts
11:20 – 11:50	Nanoparticle Engineering of Complex Fluid Behavior **Jennifer Lewis**, UIUC
11:50 – 1:00	LUNCH IN ROOM F108

SESSION VIII. MATERIALS & SIMULATIONS 2 – CHAIR: **Josef Zwanziger**, Indiana University

1:00 – 1:30	Transport, Relaxation and Structure in Nanocomposite Polymer Electrolytes **Marie-Louise Saboungi**, ANL-MSD/U. Orléans
1:30 – 2:00	Protein Folding From Big To Tiny **Yong Duan**, University of Delaware
2:00 – 2:30	Multiscale Simulations of Dynamic Fracture, Indentation, and Oxidation of Nanosystems **Rajiv Kalia**, Louisiana State
2:30 – 2:50	AFTERNOON BREAK

SESSION IX. MATERIALS 2 – CHAIR: **Ken Herwig**, ORNL-SNS

2:50 – 3:20	Crack Fronts and Damage in Glass at the Nanometer Scale **Elisabeth Bouchaud**, CEA-Saclay
3:20 –3:50	Local Structure and Long Range Order in Nanocrystalline Ceramics **Markus Winterer**, Darmstadt University
3:50 – 4:20	Ceramic Nanolaminate Multilayers **Carolyn Aita**, University Wisconsin-Milwaukee
4:20 – 4:30	WRAP UP

Saturday, March 30, 2002
PANEL DISCUSSION IN BUILDING 360 ROOM A224

PANEL MEMBERS: **Carolyn Aita, Lynn Boatner, Rajiv Kalia, Chun Loong, David Lynn and Josef Zwanziger**

9:00 – 9:15	INTRODUCTION OF PANEL – **Chun Loong**, ANL-IPNS
9:15 – 11:15	PANEL DISCUSSION
11:15 – 11:30	CLOSE OUT
11:30	MEETING ADJOURNS

POSTER PRESENTATIONS

1) **James Beitz**, Argonne National Laboratory, CHM
   Producing and Characterizing Heavy Element Nanophases in Silica
2) **Chris Benmore**, Argonne National Laboratory, IPNS
   Connectivity at the Glassy CaO-Al_2O_3 Eutectic
3) **Alok Chatterjee**, Argonne National Laboratory, IPNS
   Remote Access and Visualization of Neutron Data Using Integrated Spectral Analysis Workbench (ISAW)
4) **Ayano Chiba**, Kyoto University
   Dynamics of Liquid TeSe in the Semiconductor-to-Metal Transition Range
5) **Jijun Dong,** Emory University
   Study of Fibril Formation of Amyloid b Peptide and Metal Effect by Small Angle Neutron Scattering
6) **Lixin Fan,** Argonne National Laboratory, IPNS
   Sans Study of Structure and Interaction of Triblock Copolymer Micelles: Effects of Molecular Weight and Temperature and Sodium Carbonate Salt
7) **Chang-Ming Fang**, Eindhoven University
   Phonon Spectra and Physical Properties of Spinel-Oxides with Nano-Scale by Ab Initio Calculations and Neutron Scattering Measurements
8) **Millicent Firestone,** Argonne National Laboratory, MSD
   Ionogels: Novel Nanostructured Materials Based on Room Temperature Ionic Liquids
9) **Rex Gerald,** Argonne National Laboratory, CTD
   Thin Film NMR
10) **Catherine Han,** Argonne National Laboratory, MSD
    Preparation and Characterization of Magnetic Nanowires in Anodized Aluminum Oxide
11) **Ken Herwig,** Oak Ridge National Laboratory, ANL-SNS
    Water Mobility in Small Aerosol to Reverse Micelles
12) **Qiang Huang and Julia Chan,** Louisiana State University
    Electrodeposition and Characterization of FeCoNiCu/Cu Nanometric Multilayers
13) **Riza Kizilel,** Illinois Institute of Technology
    SANS Characterization of Fuel Cell Cathode/Ion Exchange Membranes Used in the Removal of Contaminants
14) **Alexander Kolesnikov,** Argonne National Laboratory, IPNS
    Inelastic Neutron Scattering Study of Single Wall Carbon Nanotubes Hydrogenated under High Hydrogen Pressure
15) **Wai-Tung Lee**, Oak Ridge National Laboratory, ANL-SNS
    Measurement of Lateral Ferromagnetic Domain Distribution Using Polarized Neutron Reflectometry
16) **Ken Littrell,** Argonne National Laboratory, IPNS
    The Characterization Using SANS and BET of the Controlled Production of the Pore Structure in Catalytic Carbons Prepared from Paper-Mill Sludge
17) **Ken Littrell,** Argonne National Laboratory, IPNS
    The Characterization of the Aggregation States of Tyrosine Derived Melanin Using SANS and SAXS
18) **Guokui Liu**, Argonne National Laboratory, CHM
    Confinement of Phonon Relaxation and Its Influence on Luminescence Dynamics of Rare Earth Ions in Nanophosphors
19) **Suresh Narayanan,** Argonne National Laboratory, CHM
    Probing In-Plane Distribution of Au Nanoparticles in Polymer Thin Films Using the Resonance-Enhancement Effect
20) **Amrit Panda and Elizabeth Podlaha**, Louisiana State University
    Electrodeposition of Ni-Cu-Al_2O_3 Nanocomposites
21) **Yang Ren**, Argonne National Laboratory, BESSRC CAT / MSD
    H_2 Adsorption in Carbon Nanotubes Studied with Neutron Scattering
22) **Giselle Sandi and Humberto Joachin**, Argonne National Laboratory, CHM
    In Situ SAXS Studies of Polymer Nanocomposites
23) **Suntharalingam Skanthakumar**, Argonne National Laboratory, CHM
    Local Structure of Pu Colloids in Aqueous Solutions

24) **Ken Takeuchi and Sanae Tamura,** Science University of Tokyo
Synthesis of Nano-AgI by Reverse Micelle Method

25) **Susana Trasobares-Llorente,** Rensselaer Polytechnic Institute
Time Resolved Electron Energy Loss Spectroscopy as a Tool for Controlling and Monitoring the Early Stages of Electron Beam Induced Transformations

26) **Jacob Urquidi**, Argonne National Laboratory, IPNS
Intermediate Density Amorphous Ices

27) **H. Hau Wang,** Argonne National Laboratory, MSD
Self-Assembly of OPV-PEG Based Diblock Copolymers

28) **Gerold Willing,** Argonne National Laboratory, MSD
Surface Patterning in Nanometer Dimensions: Current Capabilities and Future Directions

29) **Jean-Marc Zanotti,** Argonne National Laboratory, IPNS
Influence of Hydration and Cation Binding on a Protein Dynamics: A Study from Picosecond Up To Nasecond Time-Range

30) **Christine Rehm,** Oak Ridge National Laboratory, ANL-SNS
Hydrogen Absorption in Epitaxial W/Nb(001) And Polycrystalline Fe/Nb(110) Multilayers Studied In-Situ by X-Ray/Neutron Scattering Techniques And X-Ray Absorption Spectroscopy

31) **Frank Klose,** Oak Ridge National Laboratory, ANL-SNS
The SNS Magnetism Reflectometer: Basic Design and Neutron Guide Optimization Using Monte Carlo Simulations

32) **Josef Zwanziger,** Indiana University
The Indiana University Low Energy Neutron Source

SPEAKER ABSTRACTS

SELF ASSEMBLY AND NANOMATERIALS

Samuel I. Stupp
Board of Trustees Professor of Materials Science,
Chemistry, and Medicine
Northwestern University

A key element in nanotechnology is the synthesis of objects that can be atomically or molecularly designed for function, patterning, and interconnection. Great gaps exist at the moment in our ability to construct organic nano-objects, and self assembly of molecules offers a rich strategy toward this goal. This lecture will illustrate the use of block molecules to create zero- and one-dimensional structures that take the form of polar objects, nanoribbons, and nanofibers. Their functional value will be illustrated with examples ranging from photonic properties to nanoconductor synthesis and scaffolds for regenerative medicine. Another topic to be covered in the lecture is the use of organic objects to template inorganic structures and hybrid nanocomposites.

APPLICATION OF NEUTRON SCATTERING IN NANOTECHNOLOGY

P. Thiyagarajan
Intense Pulsed Neutron Source, Argonne National Laboratory

The nanocomposite materials, typically multi-component in nature, contain species, such as polymers, metal oxide colloids, biomaterials etc. They can be prepared as bulk materials with matrices filled by crystallites and/or pores, films, tubes and rods. These materials have complex hierarchical structures covering a wide range of length scales and it is important to obtain structural details at all length scales in order to understand their function as well as for the design of new advanced materials. The investigation of these complex systems, thus, requires a number of complementary techniques to obtain a complete picture on these systems. The key feature that makes these systems unique is the presence of structural domains with sizes in the range of 1 to 100 nm. This length scale matches well with that where SANS has the highest sensitivity. The nuclear scattering cross sections of neutrons, their low energy and higher penetration make them a versatile tool for the study of the structure and interaction in nanomaterials. The large difference in the neutron scattering cross-sections of hydrogen and deuterium provides unique contrast variation possibilities for the study of multi-component systems. In addition, the magnetic moment of neutrons enables separation of nuclear and magnetic scattering signals from which the structure of magnetic domains in these systems can be readily studied. While the SANS and Neutron powder diffraction (NPD) are powerful tools for *in-situ* studies of bulk disordered and crystalline materials, respectively, the reflectometry provides information on the layer-averaged chemical depth profiles in two-dimensionally ordered systems. In this overview talk the versatility of neutron scattering in the area of nanotechnology will be illustrated with examples.

THE SPALLATION NEUTRON SOURCE: A POWERFUL TOOL FOR NANOMATERIALS RESEARCH

Thomas E. Mason
Oak Ridge National Laboratory
Spallation Neutron Source

The wavelengths and energies of thermal and cold neutrons are ideally matched to the length and energy scales in the materials that underpin technologies of the present and future: ranging from semiconductors to magnetic devices, composites to biomaterials and polymers. In addition to the SNS ORNL is building a Center for Nanophase Materials Science that will be adjacent to the neutron facility and provide the scientific community with facilities for the preparation and characterization of materials with novel nanoscale structural features. The Spallation Neutron Source will use an accelerator to produce the most intense beams of neutrons in the world when it is complete at the end of 2005. The project is being built by a collaboration of six U.S. Department of Energy laboratories. It will serve a diverse community of users drawn from academia, industry, and government labs with interests in condensed matter physics, chemistry, engineering materials, biology, and beyond.

NANOMATERIALS AND NANOTECHNOLOGY

Richard W. Siegel
Rensselaer Polytechnic Institute
Rensselaer Nanotechnology Center and
Materials Science and Engineering Department

The past decade has seen explosive growth worldwide in the synthesis and study of a wide range of nanostructured materials, the substance of nanotechnology. A brief overview of nanoscience and nanotechnology and their relationship to novel functional materials assembled from nanoscale building blocks will be presented within the context of the U.S. National Nanotechnology Initiative and our National Science Foundation Nanoscale Science and Engineering Center for Directed Assembly of Nanostructures at Rensselaer. Several examples from our recent research results will be presented including investigations of functional nanocomposites that could find use in a variety of structural, electrical, and biomedical applications.

FROM NANOSTRUCTURED ELECTROACTIVE ASSEMBLY TO MOLECULAR P-N JUNCTION

Luping Yu
Department of Chemistry and James Franck Institute
The University of Chicago

In this talk, recent efforts on synthesis and physical characterizations of block copolymers will be presented. Many forms of structures of block copolymers will be described, ranging from coil-rod to rod-rod block copolymers. These materials were shown to self-assemble into layered, cylindrical nanostructures. Their detailed structures were characterized with various techniques. It was demonstrated that the SANS technique is particularly powerful for the characterization of the solution assembly process of these materials. Further studies showed that rod-rod block co-oligomers could be used as molecular electronic components. An example on p-n junction properties will be presented.

NANO SCIENCE AND NANO TECHNOLOGY AT ARGONNE

Axel Hoffmann
Materials Science Department, Argonne National Laboratory

Argonne National Laboratory is uniquely positioned for nano-scale research due to its combination of many exceptional characterization facilities, such as the Advanced Photon Source (APS), the Electron Microscopy Center (EMC), and the Intense Pulsed Spallation Source (IPNS). The proposed Center of Nanoscale Materials at Argonne will augment these characterization facilities with the matching tools for materials synthesis, which will be available for scientists from outside of the laboratory through a user-program. I will give a brief overview of the already existing as well as planned infrastructure, such as the nano-probe beamline at the Advanced Photon Source. This will be followed by a few selected examples of already ongoing nano-scale research at Argonne.

PROBING MAGNETIC NANOSTRUCTURES BY NEUTRON SCATTERING

S.G.E. te Velthuis
Materials Science Division, Argonne National Laboratory

Traditionally neutron scattering has been *the* tool for studying bulk magnetic materials. This success has been due to the high sensitivity of neutrons for magnetic moments, combined with the neutron's characteristics in regards to wavelength and velocity. These properties have enabled the full determination of ordered magnetic structures, detailed the mechanism of ordering and of the onset of phase transitions. As the interest of the scientific community is shifting towards nanostructured materials, techniques and tools are being developed in order to be able to investigate these new materials. Among them is the abundance of long wavelength neutrons offered by pulsed sources, and the realization that scattering at grazing incidence is sensitive to the magnetism of a few magnetic layers. I will give an overview of the scattering techniques that can be used to probe the magnetic properties of nanostructured materials by discussing experiments, among which those spearheaded at IPNS.

This work is supported by US DOE, Office of Science contract #W-31-109-ENG-38.

“SMART” AND “ACTIVE” MAGNETIC AND METAL-INSULATOR-TRANSITION NANOCOMPOSITE LAYERS FORMED BY ION IMPLANTATION

L. A. Boatner
Solid State Division, Oak Ridge National Laboratory

“Smart” surface nanocomposites consisting of an embedded layer of “active” nanometer precipitates in a host matrix represent a new materials state with unique properties. These materials are created using ion implantation and thermal processing. In these nanocomposites: each precipitate is generally a faceted single crystal that, in the case of formation in a single-crystal host, is aligned with every other precipitate. In the case of nanoparticle formation in an amorphous host, the particles are generally single crystals that may or may not be faceted and are generally not crystallographically aligned. In either single-crystal or amorphous hosts, the nanoparticles are normally physically isolated from each other by the host matrix - usually by separations whose dimensions are on the order of the nanoparticle size (i.e., there are effectively no inter-particle grain boundaries.) Compound and doped nanoparticles can be created. The “smart” nature of the near-surface nanocomposite layer arises from the use of ion implantation and thermal processing to create “active” precipitates, i.e., precipitates in which large property changes at, for example, a phase transition provide a “feedback” mechanism leading to the “smart” interaction. “Smart” and “active” embedded nanocomposite materials have several important advantages over conventional composite materials including: (1) The physical properties of the surface nanocomposite can be optimized by controlling the particle size, (2) Useful properties of two or more materials can be combined into one integrated structure by forming embedded nanocomposite layers at different depths, and (3) Embedded, active nanoparticles are protected from the environment since they are located below the surface of the host material. New physical properties and new effects in these smart nanocomposites arise from the size of the precipitates, nanophase particle-particle, and particle/host interactions. The feasibility of the “smart-surface” nanocomposite concept was initially established by the creation of several new types of optically and magneto-optically active surfaces that incorporate nanoparticles of ferromagnetic, semiconducting, and metal-insulator-transition materials in a variety of hosts. The current research objectives are: to exploit recent advances in this area by extending the conceptual approach to provide new functionalities to near-surface nanocomposites (e.g. via the formation of piezoelectric, magnetostrictive, shape memory, and other active precipitates), to understand the basic physics of these new materials, and finally, to develop new applications including thin-film and fiber-optic devices.

FERROMAGNETIC SEMICONDUCTORS AND THEIR NANOSTRUCTURES: NEW OPPORTUNITIES AND CHALLENGES

Jacek K. Furdyna
University of Notre Dame
Department of Physics

Very significant strides have recently been made in developing ferromagnetic III-V-based semiconductors (e.g., GaMnAs, InMnAs, and GaMnSb) grown in thin layer form by low-temperature molecular beam epitaxy (MBE) [1,2]. These new materials have already opened a number of fundamental issues in magnetism and magneto-transport, as well as in the inter-relationship between the two. Just as important, the development of these materials holds promise of integrating ferromagnetic (FM) and non-magnetic semiconductors, with an eye on developing new devices that depend on electron charge as well as on its spin. For example, III-Mn-V alloys have already been integrated with III-V-based non-magnetic semiconductor systems to form spin-injecting structures [3], as well as structures that allow electric-field or optical control of the ferromagnetism exhibited by the III-Mn-V alloys [4.5]. In this talk I will discuss the techniques used for fabricating and characterizing these new materials, mechanisms that underlie their ferromagnetism, the methods used to manipulate their magnetic properties (and especially their Curie temperature and coercive field), and nano-scale materials designs (such as digital alloys) which can be used to optimize ferromagnetism in this family of materials. In addition to the basic properties of ferromagnetic III-Mn-V alloys, I will also briefly review the various options for manipulating spins in semiconductor nanostructures by forming multilayer hybrids comprised of non-magnetic semiconductors and ferromagnetic systems.

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[1] H. Ohno, J. Magn. Magn. Mater. **200**, 110 (1999).

[2] J. K. Furdyna, P. Schiffer, Y. Sasaki, S. J. Potashnik, and X. Y. Liu, in *Optical Properties of Semiconductor Nanostructures,* NATO Science Series, Vol. 81, edited by M. L. Sadowski, M. Potemski, and M. Grynberg (Kluwer, Dordrecht, 2000), p. 211-224.

[3] Y. Ohno, D. K. Young, B. Beschoten, F. Matsukura, H. Ohno, and D. D. Awschalom, Nature **402**, 790 (1999).

[4] H. Ohno, D. Chiba, F. Matsukura, T. Omiya, E. Abe, T. Dietl, Y. Ohno, and K. Ohtani, Nature **408**, 944 (2000).

[5] S. Koshihara, A. Oiwa, M. Hirasawa, S. Katsumoto, Y. Iye, C. Urano, H. Takagi, and H. Munekata, Phys. Rev. Lett. **78**, 4617 (1997).

THEORETICAL INTERPRETATION OF POLARIZED NEUTRON REFLECTION AND OFF-SPECULAR SCATTERING FROM NANOCOMPOSITE FILMS

B.P. Toperverg[1,2],
[1]*Institut f. Festkoerperforschung, Forschungszentrum Juelich*
[2]*Theoretical Department, Petersburg Nuclear Physics Institute*

As well known Polarized Neutron Reflectometry (PNR) is extremely sensitive to the mean value of the neutron optical potential. It records a laterally averaged mean scattering length density profile and, correspondingly, profiles of the atomic density and magnetization distribution across the film. It is discussed how this information can be retrieved from the data either employing theoretical modelling, or in the model free way. On the other hand, nanocomposite films are, by definition, laterally heterogeneous materials and should give rise to off-specular spin-flip and non-spin-flip scattering. Close to the total reflection edge it receives significant enhancement factor and can be observed not only within the reflection plane, but also in the plane parallel to the surface. Both in-plane and out-of-plane off-specular scattering patterns carry information on the nanoparticle size distribution, correlations in their positions and magnetic moments. However, strong interaction with mean film optical potential substantially complicates quantitative interpretation of the data. In this case the Born approximation fails and one must consider not just scattering of incident neutron wave, but rather those refracted into the mean film, as well as the waves reflected from its interfaces. All this is accounted for by the Distorted Wave Born Approximation (DWBA) generalized for the case of polarized neutrons in so called Supermatrix Approach (SMA). A power of this approach is illustrated by a number of examples including treatment of the data on PNR and off-specular scattering from colloidal suspensions of magnetic nanoparticles-particles (ferrofluids), magnetic fluctuations in layered superstructures, laterally patterned films, etc. A routine based on SMA DWBA is also used to model results expected for nanocomplosite films designed by ion implantation of ferromagnetic nanocrystalls into various types of host materials. Special benefits of time-off-flight method are thoroughly discussed in view of forthcoming new powerful spallation sources.

AMYLOID STRUCTURE: MODELS AND THEORETICAL CONSIDERATIONS FOR THE CONSTRUCTION OF FIBROUS NANOSCALE SELF-ASSEMBLIES

David G. Lynn
Departments of Chemistry and Biology, Emory University
Robert E. Botto
Chemistry Division, ANL
Pappannan Thiyagarajan
IPNS Division, ANL

This presentation explores the structure of the Aβ(10-35) fibril. This central segment of the Aβ peptide of Alzheimer's Disease self-assembles into well-ordered paracrystalline arrays that seem to contradict many of the accepted paradigms established for soluble, globular proteins. Here we exploit different synthetic derivatives, solid state NMR, SANS, and initial molecular modeling efforts to assist in understanding these apparent contradictions. The emerging structure is one of a large self-assembly of β-strands, whose stability is dependent on large spatial and temporal fluctuation about a central core, giving rise to what can be best described as a dynamic and fluid tube-like micelle. This fibril structure maintains features that are distinctly different from those of either synthetic or biological fibrils, and these differences have profound implications for biomedical intervention in amyloid diseases as well as for the design of self-assembling nanoscale fibrils.

SELF-ASSEMBLED PHASES OF BIOPOLYMERS, MEMBRANES, PROTEINS, AND COUNTERIONS

Gerard Wong
University of Illinois - Urbana/Champaign

We describe the structure and interactions of a novel class of biomolecular self-assemblies, where new condensed phases of various biopolymers are formed through their interactions with oppositely charged ions of varying complexity, from point-like multivalent ions to charged amphiphilic molecules. Intuitively, two like-charged macromolecules in aqueous solution are expected to repel one another, which is essentially the prediction of prevailing mean-field theories. In the presence of oppositely charged multivalent ions, however, many biopolymers actually attract one another and condense into compact, ordered states. We have examined the global phase behavior of a large range of charged biopolymers: DNA, cytoskeletal F-actin, Fd and M13 viruses. For example, we unambiguously demonstrate the existence of two distinct condensed phases in F-actin. At low multivalent ionic strengths, a homogeneous liquid of uncondensed filaments is observed. At high multivalent concentrations, the filaments condense into uniaxial bundles, in the form of close-packed parallel arrays of individual filaments. At intermediate multivalent concentrations, however, we find a new phase of liquid crystalline matter, in the form of a multi-axial network. In contrast, cationic amphiphilic molecules can condense F-actin into hierarchically organized tubules with no direct analog in simple membrane systems. Using high resolution synchrotron small angle x-ray scattering, confocal microscopy and electron microscopies, we will present a systematic structural investigation of these condensed biopolymer phases, and the resultant implications for our understanding of polyelectrolytes, as well as a range of outstanding biomedical problems.

SUPRAMOLECULAR CHAIN REACTION

Hicham Fenniri
Purdue University

Two new hierarchical algorithms for the transfer and expression of absolute molecular chirality at the macromolecular level will be discussed. A *primer* molecule composed of the hydrogen bonding faces of the DNA bases guanine/cytosine, conjugated with 4-aminobenzo-18-crown-6-ether macrocycle on its non-hydrogen bonding face, undergoes a supramolecular chain reaction (SCR) in the presence of a molecular *promoter* to generate self-assembled nanotubes with predefined helicities, chemical and physical properties.

SCR May also be viewed as a process by which absolute molecular chirality is expressed at the macromolecular level through an auto-catalytic, programmable, stereospecific, chemoselective and hierarchical sequence of supramolecular reactions, and paves the way to the design of adaptive materials with multifaceted applications in the fields of dynamic combinatorial chemistry, materials science, and *nanochirotechnology*.

NANOSTRUCTURED MATERIALS BASED ON BLOCK COPOLYMER THIN FILMS

T. P. Russell
University of Massachusetts

Block copolymers, comprised of two polymers covalently linked at one end, self-assemble into ordered arrays of microdomains where the size scale is dictated by the size of the polymer chains, typically tens of nanometers in size. Ordered arrays of spheres, cylinders and lamellae can be obtained depending on the volume fraction of each component in the chain. Directing the self-assembly process such that the domains assume a specific orientation provides a unique route for generating scaffolds and templates for the fabrication of ordered arrays of nanoscopic structures. For example, in diblock copolymers of polystyrene (PS) and polymethylmethacrylate (PMMA) having cylindrical PMMA microdomains, by controlling interfacial interactions or by use of external fields, the cylindrical domains (10-50 nm in diameter) can be oriented normal to the surface of a thin film. Selective removal of the PMMA leaves an array of nanopores having aspect ratios that can range from 1 to 1000 with an areal density in excess of 10^{11} pores/cm^2. Evaporative or electrochemical methods can be used to fill the pores with metal, producing arrays of nanowires that have tremendous promise for magnetic storage and display applications. Copolymers of PS with poly(ethyleneoxide), on the other hand, by complexation with Li have promise as ion tranport membranes. Major advantages of the copolymer approach are the versatility in the types of copolymers, low cost, the ability to prepare these templates on virtually any substrate, the ease of producing the arrays and the robust processing conditions.

NANOPARTICLE ENGINEERING OF COMPLEX FLUID BEHAVIOR

Jennifer A. Lewis
Materials Science and Engineering Department
Chemical Engineering Department
Frederick Seitz Materials Research Laboratory
University of Illinois at Urbana-Champaign

A new mechanism for regulating the stability of colloidal particles has been discovered. Negligibly charged colloidal microspheres, which flocculate when suspended alone in aqueous solution, undergo a remarkable stabilizing transition upon the addition of critical volume fraction of highly charged nanoparticle species. Zeta potential analysis revealed that these microspheres exhibited an effective charge buildup in the presence of such species. Scanning angle reflectometry measurements indicated these nanoparticle species did not adsorb on the microspheres under the experimental conditions of interest. It is therefore proposed that highly charged nanoparticles segregate to regions near negligibly charged microspheres due to their repulsive Coulombic interactions in solution. This type of nanoparticle haloing provides a new method for tailoring the behavior of complex fluids, including its flow properties and structure.

TRANSPORT, RELAXATION AND STRUCTURE IN NANOCOMPOSITE POLYMER ELECTROLYTES*

Jacob Muthu, Emmanuel P. Giannelis
Dept. of Materials Science, Cornell University
Michel Armand
Department of Chemistry, University of Montreal
David L. Price and Marie-Louise Saboungi
Argonne National Laboratory / CRMHT, France

In this talk, we will review recent results obtained in the emerging field of nanocomposite polymer electrolytes with a special emphasis on the relaxation properties. Poly(ethylene oxide) (PEO), compounded with various salts, forms polymers with a number of potential technological applications such as advanced batteries, sensors and electrochromics.[1] In particular, Li conducting polymers are being considered as electrolytes in secondary lithium batteries that can combine high energy density with operational safety. However, their development has been hindered by the low ionic conductivities relative to molten salts or aqueous solutions.

Nanoparticles such as TiO_2 and Al_2O_3 have been reported to have a dramatic effect on ionic conductivities in $LiClO_4$-PEO solid electrolytes.[2] It is unclear whether this is due to change in crystallization kinetics or to pathways for enhanced conduction involving oxygen atoms on the surface of the nanoparticles. We have recently made structural measurements using neutron diffraction with Li isotope substitution (NDIS) and measurements of relaxation on the 10-100 nsec time scale using quasielastic neutron scattering (QENS). Careful conductivity and DSC measurements have been made on the same samples.

We will present preliminary results of these measurements and also discuss the present status of theoretical work and computer simulations on these materials.

[1] *Polymer Electrolytes*, by F. M. Gray (RSC, Cambridge, UK, 1997).
[2] B. Scrosati et al., *Nature* 1998, 394, 456

*Work supported by the Office of Science, US Dept. of Energy, under Contract W-31-109-ENG-38 and by the French CNRS.

PROTEIN FOLDING: FROM BIG TO TINY

Yong Duan
University of Delaware

All-atom molecular dynamics simulation has been an effective tool to study the folding processes of small peptides and proteins. A recent advancement has been a new set of force field parameters that takes into account the solvent polarization effect. Tests on small peptides indicate a good balance between alpha-helical and beta-sheet conformations. Results on small peptides revealed interesting folding mechanisms. Contrary to the prevailing theory on helix-formation, neither helix initiation nor helix growth cotributes significantly to the rate-limiting steps. Instead, the rate-limiting step is breaking non-native states that are stabilized by hydrophobic interactions.

MULTISCALE SIMULATIONS OF DYNAMIC FRACTURE, INDENTATION, AND OXIDATION OF NANOSYSTEMS

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This presentation will focus on large-scale (10^6-10^9 atoms) molecular dynamics simulations of dynamic fracture in nanophase ceramics and nanocomposites, nanoindentation in semiconductor and ceramic films, and oxidation of nanoparticles. Neutron scattering experiments have played an important role in these simulations, especially in the design of reliable interatomic interactions. I will also discuss the investigation of material properties and processes with a multiscale approach that combines quantum mechanical, molecular dynamics, and finite element schemes.

CRACK FRONTS AND DAMAGE IN GLASS AT THE NANOMETER SCALE

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The study of the morphology of fracture surfaces has raised a great theoretical interest in the past few years. Fracture surfaces have been shown to exhibit two self-affine regimes. The one appearing at small length scales/low average crack velocities is characterized by a roughness exponent close to 0.5. At larger length scales/higher average crack speeds, the exponent is close to 0.8. Although the values of these exponents do not vary with the material, the range of length scales where these regimes appear is very sensitive to the structure. In the case of glass, the 0.5 regime extends up to ~10nm while the 0.8 regime extends up to some 100 nm. In the case of a metallic alloy, the first regime may extend from 5nm to 30µm, and the second one up to 0.5mm.

Molecular Dynamics Simulations have suggested that glass breaks in a “ductile” way at the nanometer scale, and that the 0.5 exponent is the signature of the growth of a single damage cavity ahead of the main crack tip.

This was shown experimentally to be the case for metallic alloys.

Crack front waves propagating along the moving crack front were recently conjectured to be at the origin of this exponent. Experiments report orders of magnitude which are in fair agreement with the theoretical predictions.

However, the model has two other predictions which are currently tested: it predicts an anisotropy of the fracture surface between the directions parallel and perpendicular to the direction of crack propagation, and a roughness index 0.25 in the direction of propagation of the elastic waves.

LOCAL STRUCTURE AND LONG RANGE ORDER IN NANOCRYSTALLINE CERAMICS

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Nanocrystalline powders are produced by a modified Chemical Vapor Deposition (CVD) method where the process parameters are adjusted to produce ultrafine particles instead of films. The local structure of nanocrystalline particles and ceramics is investigated by EXAFS spectroscopy, long range order by XRD and neutron scattering. Reverse Monte Carlo (RMC) simulations make it possible to extract the complete structural information available in EXAFS spectra. Different zirconia based ceramics are used to reveal the capabilities of data analysis by RMC. EXAFS spectra provide a good "potential" for RMC in case of coarse monoclinic zirconia. RMC provides structural information independent of the initial configuration in case of an amorphous film. A comparison of the results of independent as well as simultaneous RMC analysis of neutron scattering data and EXAFS spectra of monoclinic zirconia shows the reliability of structural information obtained by the RMC analysis of EXAFS spectra. The EXAFS spectrum of a purely tetragonal zirconia powder could be fitted by a cluster model. A core-shell type structure was observed. Alumina doped zirconia was investigated by RMC/EXAFS exploiting the power of EXAFS spectroscopy to differentiate between different types of atoms by the backscattering phase and amplitude. The analysis reveals segregation at the molecular level. Measuring EXAFS spectra at the Zr and the Y K-edge and simultaneous fitting of both spectra with a single, mutual model by RMC make it possible to detect an inhomogeneous yttrium distribution in nanocrystalline zirconia doped with yttrium. The RMC/EXAFS results are consistent with the microstructural evolution of the nanocrystalline ceramics during sintering.

CERAMIC NANOLAMINATE MULTILAYERS

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In recent years, nanostructured ceramic coatings have emerged as technologically important materials chiefly because they can be tailored to exhibit unique properties and behavior not achievable in bulk. This paper addresses the design, synthesis, and characterization of tailored structures in which two or more ceramics are combined in a multilayered nanocomposite: a nanolaminate. First, we give a broad overview of the ceramic nanolaminates. We then use the sputter-deposited zirconia-alumina, zirconia-yttria, and zirconia-titania nanolaminates as model systems to discuss intralayer phase selection, interface characteristics of as-grown coatings, and architectural stability of under extreme conditions of thermal and laser annealing. Lastly, we will show how these nanolaminates can be used as components in multifunctional "smart" coatings for mechanical and corrosion protection for biomedical applications.

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POSTER ABSTRACTS

PRODUCING AND CHARACTERIZING HEAVY ELEMENT NANOPHASES IN SILICA*

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We are creating silica that contains embedded heavy metal phosphates and investigating those phases using several neutron, X-ray, and laser techniques. Small angle neutron scattering on the SAND instrument IPNS and anomalous small angle X-ray scattering on the BESSRC 12ID-C beamline at APS have proven to be particularly valuable and complementary techniques for determining the nanophase character of these materials. A chemically functionalized porous silica, termed Diphosil, into which a single type of lanthanide or actinide metal ion had been sorbed from aqueous solution, was our starting material. Heating in air decomposed the organic content of Diphosil, leaving metal phosphate and phosphoric acid in its pores. Further heating resulted in sintering, pore collapse and eventual formation of silicophosphate and crystalline metal phosphate and silica phases. Unexpectedly, the rate of pore collapse as a function of temperature and the size of the produced metal phosphate nanophases depended on the particular heavy metal ion initially sorbed into Diphosil. Hypotheses as to the underlying factors that result in the observed behavior will be presented. Some of the produced materials are candidate nuclear waste forms; others are being investigated for their unusual photophysical properties.

*This work benefited from the use of IPNS and BESSRC beam lines at APS at Argonne National Laboratory, which are funded by the Office of Basic Energy Sciences, US DOE and was carried out under the auspices of the Nuclear Energy Research Initiative and the Office of the Basic Energy Sciences of the US DOE under contract # W-31-109-ENG-38.

CONNECTIVITY AT THE GLASSY CaO-Al_2O_3 EUTECTIC.

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Calcium aluminate glasses have potential applications as laser host materials and in hydraulic cements. The total scattering of a CaO-Al_2O_3 eutectic glass has been measured over a wide momentum transfer range, using both pulsed neutron diffraction and high-energy photon diffraction techniques. The results yield high-resolution real space data on the 0.1 to 1.8 nm length scale, showing distinct molecular-type units and unit interactions. The experimental data have been interpreted through Reverse Monte Carlo simulations to help visualize the most likely unit interactions consistent with the measured intermediate range ordering in the glass. It is found that an aluminum AlO_X (where X=4,5) framework dominates the structure of the glass. The connectivity is largely determined through the interaction of a network of corner and edge sharing AlO_X units, and highly distorted CaO polyhedra.

REMOTE ACCESS AND VISUALIZATION OF NEUTRON DATAUSING INTEGRATED SPECTRAL ANALYSIS WORKBENCH (ISAW)

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With the proliferation of high intensity neutron sources and involvement of scientists from diverse areas, it is important to provide methods for remote access and display of data. We have developed an Integrated Spectral Analysis Workbench (ISAW) that can read, merge or combine, operate on, and visualize large arrays of data. ISAW is written in Java to allow it to run on common user workstations and to facilitate network communications. Recently, we added the ability to remotely access live data made available through a data server running on the control computer. Reading and writing out files in the NeXus file format is also starting to be supported.

DYNAMICS OF LIQUID TeSe IN THE SEMICONDUCTOR-TO-METAL TRANSITION RANGE

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In the solid state, both Se and Te are semiconductors that are composed of helical chains in which each atom is bonded to two adjacent atoms by covalent bonds. When Te is melted by heating, it exhibits metallic properties in contrast to Se in which the helical chain structure is more or less preserved even in the liquid state. It is well known that in liquid Te-Se mixtures a semiconductor-to-metal (S-M) transition occurs by raising the temperature and that the transition temperature increases with the Se concentration. We have carried out neutron scattering experiments on liquid Te50Se50 to study its dynamic aspects and suggested that frequent bond-switching between the chains in the metallic regime [1], as Simojo and Hoshino [2] have reported from a MD simulation for liquid Se.

Recently, the behavior of the excitations in E-Q space, such as "dispersion relation" of "optical modes", in disordered systems is beginning to be studied. In the present study, we report the evidences for the softening of "stretching modes" which indicate the strong inter-chain correlation associated with the metallic nature of these systems.

[1] A. Chiba, Y. Ohmasa, M. Yao, O. Petrenko and Y. Kawakita, J. Phys. Soc. Jpn. 71 (2002) 504.
[2] F. Shimojo, K. Hoshino, M. Watabe and Y. Zempo, J. Phys.: Condens. Matter 10 (1998) 1199.

STUDY OF FIBRIL FORMATION OF AMYLOID b PEPTIDE AND METAL EFFECT BY SMALL ANGLE NEUTRON SCATTERING

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David M. Morgan, Robert P. Apkarian, Jaby Jacob
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Under certain conditions, small peptides can self-assemble to form long ordered supra-molecular fibrils, among them is included the amyloid β peptide (Aβ) and its derivatives. Full-length amyloid β peptides (Aβ) with 42 amino acids self-assemble to form unbranched, twisted or flat fibrils 100Å wide and several micrometers long. By shortening the peptide length or changing the solution conditions, the fibril morphology shown by electron microscopy is variable and controllable. Based on solid state NMR and small angle neutron scattering experiments, we have proposed a molecular model of the fibrils formed by Aβ(10-35), which is identical in primary sequence and fibril morphology to full-length amyloid β peptide. In this model, extended parallel β strands, perpendicular to the direction of the fibril axis, are stacked to form extended sheets 80Å wide and with each amino acid residue in exact register. The β-sheets are laminated six deep in the perpendicular dimension giving fibril of a 60Å in depth.

Understanding the contributions of various factors that stabilize the fibril structure, especially on the lamination dimension, is important to control peptide self-assembly into fibrils with expected structure and function. In the poster we discuss the role of Zn^{2+} in controlling both fibril assembly and morphology, characterized by electron microscopy and small angle neutron scattering. We also proposed to put alkanethiol-attached amyloid β peptides to a gold surface, which may form an ordered monolayer structure. Such an ordered array will contribute to an understanding of fibril structure and put further limits on the nature of the laminate energies.

SANS STUDY OF STRUCTURE AND INTERACTION OF TRIBLOCK COPOLYMER MICELLES: EFFECTS OF MOLECULAR WEIGHT AND TEMPERATURE AND SODIUM CARBONATE SALT

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We have investigated the micellization and interaction in aqueous solutions of triblock copolymers of 5 wt.% F38, F68, F88, F98 and F108 using small angle neutron scattering as a function of temperature and concentration of sodium carbonate. The critical micellization temperatures and concentrations and the thermodynamic parameters of micellization were obtained for F108 in presence of salt. SANS data were fitted by using appropriate form factor and structure factors to extract the information on the size of the core, corona, inter-particle distance, aggregation number and the volume fraction of the micelles. These studies show that the temperature, molecular weight of the triblock copolymers and sodium carbonate have a strong effect on the micellization. As the molecular weight increases, the micelle aggregation number and the radii of the core, corona and hard sphere increase. However, the temperature at which the saturation of the volume fraction of the micelles (completion of the micellization) decreases with increasing molecular weight. Presence of sodium carbonate decreases both CMT and the temperature transformation from unimer and micelle coexist to full micelle as well as spherical to cylindrical micelles occurs. Furthermore, the micellization and transition temperatures decrease with increasing molecular weight of the copolymer as well as the salt concentration. The mechanism of the micellar structure and the phase separation is through gradual dehydration of the copolymer chains with an increase in either the temperature and/or the salt concentration. Progressive dehydration occurs in the core at lower temperature, whereas progressive insertion of PEO units in to the core occurs at higher temperature (T>50 ^{o}C).

PHONON SPECTRA AND PHYSICAL PROPERTIES OF SPINEL-OXIDES WITH NANO-SCALE BY Ab INITIO CALCULATIONS AND NEUTRON SCATTERING MEASUREMENTS

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G. A. de Wijs and G. de With

A variety of inorganic compounds have the spinel-type structure and show many particular physical properties and applications. The spinels have layered structure along different orientations and many possible terminations (or surfaces) along each orientation. Both theoretical calculation approaches, including ab initio Density-Functional Theory (DFT) and classic pair-potential method with slab- and/or supercell approximations, and experimental techniques, particular neutron scattering, are applied to zero- (clusters) and two- (surfaces) and three-dimensional (bulk) systems. Strong structure relaxation or even reconstruction due to dimensional changes (quantum confinements) and surface compositions and the correspondingly changing physical properties, are addressed. The methods have been given to spinels such as $MgAl_2O_4$, $ZnAl_2O_4$ and recently discovered cubic Si_3N_4.

IONOGELS: NOVEL NANOSTRUCTURED MATERIALS BASED ON ROOM TEMPERATURE IONIC LIQUIDS*

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Room-temperature ionic liquids (RTILs) have attracted much recent interest as potential replacements for conventional organic solvents in a variety of applications, a result of a number of favorable physicochemical properties, among them high boiling points, low vapor pressures, and wide electrochemical windows. Previous studies have shown that certain long-chain (n=12 or greater) 1-alkyl-3-methylimidazolium salts form liquid crystalline phases at elevated temperatures. In this work, we demonstrate that by addition of an appropriate co-solvent, short-chain imidazolium salts can be induced to form ordered phases at room temperature. The results of calorimetric, spectroscopic, and small-angle X-ray scattering studies of these novel mesophases are presented.

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THIN FILM NMR

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We have investigated self-assembled thin films of dodecanethiol on atomically flat mercury surfaces by proton NMR spectroscopy. At room temperature, we observed a single broad peak (1 ppm line width at half height) with an anomalous chemical shift of –4.1 ppm. Nutation of the proton magnetization showed that the signal originates from a very narrow region of space where the radiofrequency magnetic field is the most intense. Spin-lattice relaxation rate measurements of the magnetization were fitted to a mono-exponential curve ($1/T_1 = 1\ s^{-1}$). The spectrum showed no variation with decreasing temperature from 23 °C to approximately the freezing point of mercury (-39 °C), at which point the signal abruptly vanishes. The results are consistent with our view that the alkane chains are rapidly interchanging positions on the liquid mercury surface. The intermolecular dipolar interactions between methylene protons are removed by translational chain mobility on liquid mercury, but severely broaden the spectrum when chain mobility is halted on solid mercury. We will present our latest experimental NMR data, and describe the novel detector used to record NMR spectra and images of the thin films. We will also discuss scattering experiments performed on the same system by other workers. This work was supported by the U.S. Department of Energy, Division of Chemical Sciences, Office of Basic Energy Sciences, under Contract W-31-109-Eng-38.

PREPARATION AND CHARACTERIZATION OF MAGNETIC NANOWIRES IN ANODIZED ALUMINUM OXIDE

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Anodized aluminum oxide (AAO) films with pore diameters ranging from 10 nm to 200 nm were prepared by multistep anodization in oxalic, sulfuric and phosphoric acids under varied reaction conditions. The nanochannel arrays of AAO films were characterized with use of SEM, AFM, and SAXS analyses. SEM analysis showed the largest ordered domain with hexagonally closed packed nanochannels was ~ 2.5 µm by 2.5 µm. Porous magnetic thin films of Ni and Fe_3O_4 (~100 nm thick), and magnetic nanowires of Co and Ni with diameters ranging from 20 nm to 200 nm were prepared by electrodeposition with commercial and synthesized AAO membranes. Growth of nanowires in both aqueous and organic solution (dimethyl sulfoxide, DMSO) was carried out successfully and better quality nanowires were obtained from DMSO solution. The structure and magnetization hysteresis of the nanowires imbedded in AAO membranes were investigated with SEM and SQUID. The influence of the diameter, the length of the nanowires and the distances between nanowires on the magnetization anisotropy will be presented.

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WATER MOBILITY IN SMALL AEROSOL TO REVERSE MICELLES

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Reverse micelles are nanoscale droplets of polar solvent surrounded by a surfactant layer in nonpolar solvents. We have used quasielastic neutron scattering to investigate the mobility of water molecules in small reverse micelles. Rotational reorientations have been probed using the QENS spectrometer at the IPNS facility at Argonne National Laboratory, for water/surfactant ratios of 1, 2.5, and 5. Translational motion within the droplets has been investigated at higher ratios using the new disk chopper spectrometer at the NIST Center for Neutron Research. Preliminary analysis indicates that reorientations of the water molecule are both slower and more geometrically restricted in the low ratio samples.

ELECTRODEPOSITION AND CHARACTERIZATION OF FeCoNiCu/Cu NANOMETRIC MULTILAYERS

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At present, nanometric multilayers composed of alternating ferromagnetic and nonmagnetic materials are used as components in hard disk drives. The compositional layering induces giant magnetoresistance (GMR), which refers to a change of resistance in the presence of a magnetic field. As storage bit density increases greater head sensitivities are a necessity, which is the motivation for our work. Despite the promise of reported multilayered FeCoNi/Cu films fabricated by magnetron sputtering exhibiting GMR in low fields, no studies to our knowledge have examined the analogous electrodeposited system. In our study, FeCoNiCu/Cu multilayers were fabricated by electrodeposition and characterized with X-ray fluorescence (XRF), X-ray diffraction (XRD), and transmission electron microscopy (TEM) with selected area electron diffraction (SAED). A GMR effect was measured using the standard 4-probe AC technique. Nanometric multilayer structures with layer thickness at about 10 nm was verified by TEM and SAED and showed both FCC and BCC phases. For multilayers below 10 nm, on the order of a nanometer, the preferred orientation of the crystallographic structure was found to be a function of the layer size. The structure was also correlated with the GMR property. A maximum GMR of 6% was found when the calculated Cu and alloy layer size was 1.8 and 2.0 nm, respectively.

SANS CHARACTERIZATION OF FUEL CELL CATHODE/ION EXCHANGE MEMBRANES USED IN THE REMOVAL OF CONTAMINANTS

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Contaminants in hard chromium bath is one of the major problems for both the process and the environment. In this work, a fuel cell cathode/ion exchange membrane (FCMP) was used to remove the contaminants continuously from hard chrome plating bath and the results were verified experimentally on a laboratory scale. The membranes were composed of a mixture of platinum-carbon (Pt-C) embedded on a Nafion surface. At room temperature and at constant current, this study indicates the feasibility of the FCMP process and its potential benefits when integrated into industrial-scale plating operations. Energy savings in the separation of contaminant metals and continuous regeneration of the plating bath are principal benefits of the FCMP process. The Pt-C structural changes were monitored using SANS. The changes in the carbon structure proved to be detrimental in the membrane performance.

This work was performed under the auspices of the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Chemical Sciences, Geosciences and Biosciences, under contract number W-31-109-ENG-38

INELASTIC NEUTRON SCATTERING STUDY OF SINGLE-WALL CARBON NANOTUBES HYDROGENATED UNDER HIGH HYDROGEN PRESSURE

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Carbon nanotubes is one of the most exciting molecular systems at present because of their large potential for nano-scale technological applications and the prospects for hydrogen storage. Besides the application importance, the material is very attractive for the fundamental research due to its unique crystal structure.

In the present work the single-wall carbon nanotubes (SWNT) were hydrogenated at a hydrogen pressure of 30 kbar and 620 K, quenched to 80 K and then studied by inelastic neutron scattering (INS) in a wide range of neutron energy transfers, 3-400 meV. INS was measured using the TOSCA-II spectrometer (ISIS, RAL) first on the hydrogenated and quenched sample and then on the same sample annealed at 332 and 623 K. All INS data were collected at 15 K. The obtained spectra show that the quenched sample has hydrogen covalently bound to the carbon atoms (thus revealing that the sample is constructed of new SWNT&H "macromolecules") and molecular hydrogen on interstitial positions. The greater part of H_2 molecules (~65%) left the sample after the first annealing at 332 K, but the rest H_2 molecules (~35%) still stayed in SWNT&H. Final evolution of the H_2 molecules from the sample occurred upon the second annealing at 623 K. The data obtained from the quenched sample on the eVS spectrometer at ISIS showed that the total atomic content of hydrogen was x = H/C = 0.345 ± 0.008 (or 2.88 ± 0.07 wt%).

This is the first INS study of SWNT&H (with covalently bound hydrogen) with and without molecular hydrogen on interstitial positions. The obtained INS spectra are compared with those for hydrogenated C_{60} fullerites prepared in rather similar ways, but having different crystal structures (bcc or fcc) and different H contents in hydrofullerite molecules $C_{60}H_x$, x = 24, 32 and 36.

The bending C-H modes in the INS spectra show a broad structured peak at 140 to 173 meV for hydrofullerites and two individual peaks at ~146 and 167 meV for SWNT&H. The analysis of the two-phonon band between 280 and 340 meV in the INS spectrum of SWNT&H shows that two peaks in the bending mode range originate from neutron scattering on the same hydrogen atoms. Thus we can conclude that covalently bound hydrogen atoms occupy equivalent positions in SWNT&H sample (more probably, on the outer surface of the tubes, exohydrogenated SWNT).

The spectral components related to neutron scattering on molecular H_2 are different for H_2 in SWNT&H and $C_{60}H_x$. The INS spectrum of H_2 in SWNT&H has a relatively narrow main peak at 14.3 meV (close to the $J=0 \rightarrow J=1$ transition for the free H_2 rotor). The H_2 spectrum of $C_{60}H_x$ has two broad peaks with maxima at about 10 and 16 meV for x=36 and at 9 and 15 meV for x=32. In addition, these spectra include a broad intense peak at ~31 meV attributed to the $J=1 \rightarrow J=2$ transition due to the presence of the ortho-hydrogen molecules (o-H_2). No peaks were observed around this energy in the spectrum of H_2 in SWNT&H, which indicates that the amount of o-H_2 in the quenched sample is negligible. The present data are discussed also in relation to the earlier INS studies of molecular H_2 absorbed in pure SWNT and pure C_{60}.

MEASUREMENT OF LATERAL FERROMAGNETIC DOMAIN DISTRIBUTION USING POLARIZED NEUTRON REFLECTOMETRY

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It is well known that in polarized neutron reflectometry (PNR) magnetic moments perpendicular to the neutron polarization axis give rise to the spin-flip intensities. It has, however, long been overlooked that the spin-flip reflectivities also measure the distribution of lateral magnetic domains across a thin film. We will show how PNR can determine in a model-free way not only the mean magnetization of a ferromagnetic thin film at any point of a hysteresis cycle, but also the mean square dispersion of the magnetization vectors of its lateral domains. This technique is applied to elucidate the mechanism of magnetization reversal of an exchange-biased Co/CoO bilayer. The reversal process above the blocking temperature Tb is governed by uniaxial domain switching, while below Tb the reversal of magnetization for the trained sample takes place with substantial domain rotation.

THE CHARACTERIZATION USING SANS AND BET OF THE CONTROLLED PRODUCTION OF THE PORE STRUCTURE IN CATALYTIC CARBONS PREPARED FROM PAPER-MILL SLUDGE

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Activated carbons play an important role in many areas of modern science and technology such as purification of liquids and gases, separations of mixtures, and catalysis. Their value for any particular application is determined by the characteristics of their pore structure. In this study we have used small-angle neutron scattering (SANS) and N2-BET to characterize the microstructure of a series of activated carbons produced from paper mill sludge using different amounts of $ZnCl_2$ as the chemical activating agent. The size and morphology of the pores and inclusions were determined from the SANS data. The pores in these carbons are roughly rod-like with radii and volumes that increase as the amount of $ZnCl_2$ used for the production of the carbons increase. Contrast-variation SANS studies demonstrate the existence of two different phases, a zinc-rich particle phase and a bulk carbon phase with nanopores. Both phases are accessible to the solvent. Based on these results, we propose a conceptual model describing these carbons as consisting of amorphous carbon containing zinc-rich particles in large voids linked by narrow channels.

This work has benefited from the use of the Intense Pulse Neutron Source at Argonne National Laboratory, and was performed under the auspices of the U.S. Department of Energy, Office of Basic Energy Sciences; Division of Chemical Sciences, under contract number W-31-109-ENG-38.

THE CHARACTERIZATION OF THE AGGREGATION STATES OF TYROSINE-DERIVED MELANIN USING SANS AND SAXS

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Melanin, the ubiquitous pigment that imparts color to the hair, skin and eyes in humans and animals, plays an important role in a highly evolved photobiological protection system. It filters the wavelengths of light roughly in proportion to their ability to cause actinic damage to tissue and it is able to scavenge and neutralize a variety of free radicals. The photoprotecive properties of melanin vary with its type, which, in turn, is dependent on its structure. In this study we have used small-angle x-ray scattering to probe the structure of a series of aggregation states of tyrosine-derived melanin bleached with H_20_2; the results are interpreted in terms of a melanin protomolecule model. At normal pH values in the absence of metal ions the melanin particles are best described as thin disks or oblate ellipsoids, consistent with the model of a planar aggregate of six to ten nanometer-sized melanin protomolecules which are hydrogen-bonded across their quinone and phenolic perimeters. As the concentration of H_20_2 used to bleach the increases, the radius of the melanin particles decreases while their thickness remains nearly constant. We interpret this deaggregation as evidence for oxidative disruption of hydrogen bonds between protomolecules.

This work was performed under the auspices of the U.S. Department of Energy, Office of Basic Energy Sciences; Division of Chemical Sciences, under contract number W-31-109-ENG-38.

CONFINEMENT OF PHONON RELAXATION AND ITS INFLUENCE ON LUMINESCENCE DYNAMICS OF RARE EARTH IONS IN NANOPHOSPHORS

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We report observation and theoretical analysis of an anomalous thermalization effect induced by optical excitation of Er^{3+} in nanocrystals of Y_2O_2S. Due to absence of low-energy phonon modes in 20-40 nm crystals, the nonradiative multiphonon relaxation between electronic states with energy gaps less than 100 cm^{-1} is significantly diminished, while the confinement on high-energy phonon relaxation and thermalization is negligible. As a result, the intensity of hot bands originating from the upper crystal field levels in the $^4I_{15/2}$ ground state increases abruptly as temperature decreases below 8 K, and the ground level Er^{3+} population can be deeply depleted by a 5-ns laser pulse of 100 W/mm^2. This anomalous thermalization effect is interpreted satisfactorily based calculations of temperature dependent multiphonon relaxation rates in nanocrystals of confined phonon modes. Our theoretical analysis provides in general a fundamental understanding of phonon confinement effect on luminescence dynamics of rare earth ions in nanocrystals, which was also observed previously in nanocrystal of Eu_2O_3 when the $^7F_1$ to $^5D_1$ hot bands at 12 K became significant in the crystals with diameters less than 10 nm. Some related effects such as confinement on phonon-assistant energy transfer are also to be discussed. Work performed under the auspices of DOE BES, Division of Chemical Sciences under contract No. W-31-109-ENG-38.

PROBING IN-PLANE DISTRIBUTION OF Au NANOPARTICLES IN POLYMER THIN FILMS USING THE RESONANCE-ENHANCEMENT EFFECT*

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Dispersions of metal nanoparticles in polymeric matrices are of importance in the field of nanoscience. To study the dynamic and structural properties of nanoparticles in ultra thin polymer films, we have developed a method involving resonance-enhanced small-angle scattering and diffuse scattering by nanocomposite thin films. Previously, the resonance-enhancement effect of a x-ray beam impinging upon a thin-film surface at a grazing-incident angle has been recognized as a x-ray wave-guiding phenomena. In the present study, diffuse scattering by gold nanoparticles embedded in ultra thin polymer films (coated on x-ray reflecting mirrors) was found to exit the polymer films in a resonance-enhanced manner at a few discrete grazing angles (in various guided modes). In order to study the in-plane structure of the nanocomposite systems, grazing-incidence small-angle x-ray scattering (GISAXS) measurements have been carried out using such an enhancement effect. The dynamics of the lateral diffusion of Au nanoparticles above the glass transition temperature of the polymer have also been studied.

Acknowledgments: The measurements were carried out at 1-BM beamline at the APS. *This work and the use of the APS are supported by the U.S. Department of Energy, under contract W-31-109-ENG-38.

ELECTRODEPOSITION OF Ni-Cu-Al_2O_3 NANOCOMPOSITES

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Electrodeposited nanocomposites are of interest for both thin and thick film applications. Ceramic nanoparticles dispersed in metal matrices have been found to improve the tribological and mechanical properties of the deposit. In this study, the electrodeposition of Ni-Cu alloys with and without γ-alumina nanoparticulates from a citrate electrolyte are investigated. Our interests in electroformed Ni-Cu metal matrices are motivated by their exceptional corrosion resistance compared to nickel and the translation of this electrodeposition process into deep recesses to expand materials available for microdevice fabrication. Deposition experiments were performed on rotating cylinder electrodes and recessed microelectrodes 500 μm thick. Recessed electrodes were produced by x-ray radiation at the LSU synchrotron facility, the Center for Advanced Microstructures and Devices (CAMD). The concentration of copper in the electrolyte was much lower than the nickel concentration, ensuring that it is under mass transport control for most applied currents. In the microstructure, the copper concentration in the deposit was found to increase with the addition of alumina nanoparticles in the electrolyte. This rate enhancement of the diffusion-limited copper can be attributed to improved agitation in the recess provided by the alumina nanoparticles. The results of this study suggest a novel use of nanoparticulates: to enhance the metal reaction rate in deep cavities for the development of microdevices as well as yielding an improved material through the incorporation of the particle.

H_2 ADSORPTION IN CARBON NANOTUBES STUDIED WITH NEUTRON SCATTERING

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H_2 adsorption in single-walled carbon nanotubes (SWCNTs) has been studied with quasielastic and inelastic neutron scattering. At 80 K, under a H_2 pressure of 110 atm, H_2 molecules gradually condense in the SWCNT sample. After pumping out at 25 K and 20 mTorr, the remaining H_2 molecules show a quantum rotational transition at 14.560.1 meV, with a peak width that increases linearly with increasing temperature from 4.2 to 35 K. The H_2 molecules remain in the sample up to 65 K and then start to desorb with increasing temperature. A broad inelastic scattering spectrum from the adsorbed hydrogen is also observed. The time scale of the dynamics is longer than 15 ps even at 200 K. Our results imply that hydrogen molecules are physisorbed in the interstitial tunnels of the SWCNT bundles.

IN SITU SAXS STUDIES OF POLYMER NANOCOMPOSITES

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A series of nanocomposites containing polyethylene oxide (PEO) intercalated in the layers of synthetic lithium hectorite (SLH) clays have been prepared. Isomorphous substitutions in the lattice of Li(I) for Mg (II) in the octahedral layers of hectorite cause an overall negative charge that is compensated by the presence of interlayer, or gallery, cations. In the case of SLH, these are lithium (I) cations. Preferential orientation in films prepared by natural occurring clays tends to occur. This can lead to non-conducting planes being perpendicular to the current path and thus reducing the conductivity. To avoid these problems, we developed a method which involves direct hydrothermal synthesis and crystallization of the clay mineral from a gel. Novel clay assemblies result from this method. PEO is incorporated afterwards via an aqueous immersion. In situ SAXS temperature dependence studies indicate that the polymer is incorporated in the clay layers and the clay structure remains intact upon heating.

This work was performed under the auspices of the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Chemical Sciences, Geosciences and Biosciences, under contract number W-31-109-ENG-38.

LOCAL STRUCTURE OF Pu COLLOIDS IN AQUEOUS SOLUTIONS

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It has been demonstrated that high-energy X-ray scattering, in combination with X-ray absorption spectroscopy (XAS), can used to determine unique structural information about small, colloidal metal particles in solution. The example chosen for discussion involves Pu^{4+} ions which, in a slightly acidic aqueous solution, aggregate to form colloids. Earlier X-ray diffraction and electron microscopy studies found there to be two different colloid phases after drying – an amorphous phase and a crystalline phase. The crystalline dried phase had a Fm3m structure consistent with bulk PuO_2. Our conventional diffraction experiments reveal a significant difference in the patterns obtained before and after drying. The data from the solution sample do not exhibit well defined diffraction lines. In order to probe Pu atomic correlations <u>in solution</u>, we used a combination of high-energy (115 keV) X-ray scattering and X-ray absorption spectroscopy (XAS). Pair distribution functions (PDF)s obtained by Fourier transforming (FT) the scattering data show well defined correlations out to distances of almost 20 Å. The distances of the atomic correlations are similar to those produced by crystalline PuO_2. The PDF data also contains information on colloid size that permits the estimation of a particle size of 20 Å <u>in solution</u>. This result is consistent with previous electron-microscopy studies on the amorphous colloidal component. Overall, the results are consistent with only one colloidal component in solution. The implications of these experiments for the structural identification of small colloids and nanoparticles will be emphasized.

This work has benefited from use of the Actinide Facility and the Advance Photon Source, and is supported by the U. S. DOE, Basic Energy Sciences, Chemical Sciences, under contract W-31-109-ENG-38.

SYNTHESIS OF NANO-AgI BY REVERSE MICELLE METHOD

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α-AgI is one of the best-known highly conducting solid electrolytes. Under atmospheric pressure, β-AgI has a phase transition to α-AgI at 147 °C. Comparing nanoparticle with the bulk material, it is expected that the phase transition temperature for nano-AgI can be lowered. We used the reverse micelle method to synthesize nano-AgI particles. The ternary system alkane/AOT/water produces monodisperse spherical reverse micelles with "water pool" at their core. The radius of the water pool is controlled by the ratio of water to surfactant concentration. The chemical reaction and co-precipitation between reactants solubilized in two different reverse micelles are carried out under controlled environment. In order to correlate the property of the nano-AgI particles and the environments in which they are synthesized, we used small angle neutron scattering (SANS) and TEM for the characterization of systems involved in their synthesis.

In this study, nano-AgI was prepared by mixing two kinds of the microemulsions containing $AgNO_3$ *aq.* and KI *aq.* These aqueous solutions formed the cores of the reverse micelles. Each microemulsion consisted of organic solvent (*n*-heptane or toluene), surfactant (AOT), and above mentioned aqueous solutions.

We investigated the structure of reverse micelles with w=2, 8, and 16 prepared by using deuterated *n*-heptane or deuterated toluene at room temperature in order to study the core-shell structural changes due to different w and different solvents.

We also studied the temperature dependence of the size of the reverse micelle (w=8) by measuring SANS for solutions at 9, 20, 28, and 70 °C. The radius of the micelles, shell thickness and water pool core radius decreased with increasing temperature and the changes were reversible with temperature. The particle diameters derived by TEM of the powders were generally larger than those estimated from water core radii from SANS.

TIME RESOLVED ELECTRON ENERGY LOSS SPECTROSCOPY AS A TOOL FOR CONTROLLING AND MONITORING THE EARLY STAGES OF ELECTRON BEAM INDUCED TRANSFORMATIONS

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Spatially Resolved Electron Energy Loss Spectroscopy (EELS) in the context of a Scanning Transmission Electron Microscope (STEM) has been demonstrated to be a powerful technique for studying the chemistry and electronic structure of materials at the nanometer scale. Most recent developments on the acquisition system have highly improved the sensitivity of the technique, as clearly demonstrated by selective atoms imaging [1]. The high detention efficiency of the charged coupled device (CCD) camera detector offers new possibilities to the EEL spectroscopy. With the new system, the required acquisition time for recording a satisfactory signal has been brought down to 10 to a few 100 ms for the core loss region (i.e. on the C or N Kedge). These improvements provide the possibility of studying the early stages of beam induced specimen transformation, by monitoring the Energy Loss Near Edge Structures (ELNES) changes using Time Resolved EELS (chrono-spectroscopy mode). Moreover the combination of Time and Spatially Resolved EELS with adapted mathematical methods, like Multivariate Statistical Analysis (MSA), allows us to control and monitor in situ in the electron microscope the electron beam induced transformations. In the chrono-spectroscopy mode, a probe of 0.5 nm in diameter with a current of *ca* 0.15-0.20 nA is fixed at a specific location on the specimen and a series of spectra are recorded with the dose as variable (with roughly dose = time x 10^9 e^-/nm^2 s). In this paper, we illustrate this technique by studying the beam-induced processes in two different systems:

Electron beam induced processes on melamine.

Melamine is highly sensitive to radiation damage, visual changes are observed in the analysed area as soon as the electron beam is focused on the system. Time Resolved EELS data reveals C and N losses during the process, with a 40% decrease on the N/C ratio being observed. Monitoring ELNES shows that a strong p* peak at the carbon edge, which is observed at the beginning of the process, strongly decreases when the total applied dose is approximately 10^{11} e^-/nm^2. For the N K edge, the situation is more complex, the appearance and vanishing of several peaks at the onset of the N K edge are observed during the process. A clear peak at 401.1eV, which has being associated to the presence of N_2 gas, is observed when the applied dose is $4x10^8$ e^-/nm^2. From the comparison of experimental data with simulated spectra obtained using molecular orbital theory, we suggest that the amino groups are first eliminated and N_2 gas is released as one of the decomposition products. Then the degradation of the molecule occurs through a reduction of the carbon-nitrogen double bonds. If the irradiation is maintained over longer periods the formation of different CN fragments and polymerisation products may happen [2].

Controlling and monitoring electron beam induced process on nitrogen doped nanotubes.

Spatially resolved EELS on carbon nanotubes produced by catalytic pyrolysis of camphor provides the first experimental evidence of trapping N_2 in the cavity of the nanotube during the synthesis process. Performing chrono-spectroscopy on these nano-structures, we have monitored and controlled the produced changes under electron beam irradiation. CN_x nano-islands (20 nm in diameter) have been regularly produced all along the nanotube by puncturing the walls of the nanotube, releasing most of the trapped gas and gradually incorporating the remained nitrogen into the previously amorphised carbon system [3].

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INTERMEDIATE DENSITY AMORPHOUS ICES

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Ice is known to have at least two reproducible amorphous phases produced by compression of crystalline ice Ih: high density amorphous (HDA) ice and low density amorphous (LDA) ice. Here we report the discovery of several intermediate amorphous ice phases, obtained by annealing H_2O-HDA ice at different temperatures for several hours. Structural measurements were performed using pulsed neutron and high-energy x-ray diffraction techniques. Five amorphous phases were characterized by the position of the first peak in the static structure factor, S(Q), at temperatures between 40K and 115K. The new structures could not be reproduced by any combination of the known HDA and LDA ice phases. The results suggest that a continuum of metastable ices exist between the widely accepted HDA and LDA states.

SELF-ASSEMBLY OF OPV-PEG BASED DIBLOCK COPOLYMERS

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During the past few years, we have elucidated the molecular packing of OPV-PEG based nanofibers where OPV is oligo(phenylenevinylene) and PEG is poly(ethyleneglycol). These diblock copolymers undergo self-assembly in organic solvents to form long rod-like cylinders with photoluminescent OPV inner cores and PEG outer shells. These nanofibers can be filtered from solutions and directly observed with use of TEM techniques. Typical radii of these fibers are around 8 nm determined from small angle neutron scattering. Recently, we discovered that the OPV-PEG based di-block copolymers form a new lamella structure in the melt. These block copolymers were studied using SAXS at the Advanced Photon Source. For OPV_{13}-PEG_{13}, where 13 indicates the number of repeating monomer units, a layer-to-layer distance of 12.8 nm was directly measured. For OPV_{13}-PEG_{114}, a layer-to-layer distance of 25.0 nm was observed. The packing motifs of these novel materials will be presented. These layered materials consist of alternating photoluminescent OPV layers. The implication of photonic application with these nanostructured materials will be discussed.

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SURFACE PATTERNING IN NANOMETER DIMENSIONS: CURRENT CAPABILITIES AND FUTURE DIRECTIONS

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The development of techniques for the creation of reproducible, predefined surface patterns on the nanoscale has seen an increase in research activity over the past several years. This is due, in no small part, to increased interest in the effects of nanoscale confinement in photonics, magnetics and electronics. Though many techniques are currently being investigated, dip-pen nanolithography (DPN) and polydimethylsiloxane (PDMS) stamping are among those that can be performed with relative ease. Through the use of these two techniques, alkane thiols with a variety of chain end functionalities can be patterned directly onto smooth gold surfaces. These chemical patterns can then be used as templates for material deposition or predefined crystal growth. As both techniques are still in the early stages of development, the current capabilities of each, along with their potential applications, will be discussed.

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INFLUENCE OF HYDRATION AND CATION BINDING ON A PROTEIN DYNAMICS: A STUDY FROM PICOSECOND UP TO NASECOND TIME-RANGE

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Hydration, internal dynamics and function in proteins are intimately associated [1]. Parvalbumins are acidic Ca^{2+} and Mg^{2+} binding proteins of 11.5 kDa with two Ca^{2+} / Mg^{2+} binding sites [2]. They belong to the EF-hand superfamily and are ubiquitous in vertebrates. Through its properties of Ca^{2+}/ Mg^{2+} exchange, parvalbumin is associated with muscle and neuron relaxation after excitation by Ca^{2+}.

The increase of the quasi-elastic signal observed, upon hydration, by neutron scattering, has been interpreted as an increase of the local mobility of side-chains protons, mainly of the hydrogen rich lysyl residues (17 residues over 109). This result was in agreement with those from a parallel study of solid-state natural abundance ^{13}C cross-polarization and magic angle spinning NMR. It was shown [3] that the dynamics of surface charged residues in the picosecond time range, as seen by neutrons, was concomitant with the dynamics of the protein backbone, in the nanosecond time range, as seen by NMR.

In the present work, we take advantage of the complementarities in energy resolution of various neutron spectrometers (time of flight, backscattering, spin-echo) to extend our previous neutron measurements. We probe the parvalbumin dynamics from a fraction of picosecond to a few nanoseconds.

Influence of hydration and of the nature of the cation on parvalbumin dynamics are discussed.

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HYDROGEN ABSORPTION IN EPITAXIAL W/NB(001)- AND POLYCRYSTALLINE FE/NB(110) MULTILAYERS STUDIED IN-SITU BY X-RAY/NEUTRON SCATTERING TECHNIQUES AND X-RAY ABSORPTION SPECTROSCOPY

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Hydrogen can be absorbed in large quantities by thin Nb layers (20-1000 Å) embedded in epitaxial W/Nb and polycrystalline Fe/Nb multilayers. The hydrogen-induced structural changes of the host lattice are explored in-situ by small-angle X-ray reflectometry and high-angle diffraction. These measurements reveal for both systems that the relative expansion of the Nb layers is considerably larger than the relative increase of the Nb interplanar spacing indicating two distinctly different mechanisms of hydrogen absorption. For Fe/Nb, hydrogen expands the Nb interplanar spacing in a continuous way according to the external pressure. In-situ X-ray absorption spectroscopy shows that this process is discontinuous for epitaxial W/Nb. Up to p_{H2} = 1 mbar, the Nb layers expand only in the out-of-plane direction. After applying this pressure over a period of several hours, both in- and out-of-plane Nb/Nb distances transform into a considerably expanded phase.

Hydrogen concentration measurements are carried out in-situ by small-angle neutron reflectometry in order to measure the film thickness dependence of the solubility isotherms at 185°C. For small Nb film thickness, the curves are shifted by several orders of magnitude to higher hydrogen pressures. The experiments reveal further that hydrogen can not easily be removed from the films by lowering the external pressure. Large amounts of hydrogen remain in both the epitaxial W/Nb and polycrystalline Fe/Nb multilayers.

There is an important effect of hydrogen on the magnetic properties of Fe/Nb multilayers. As we have shown recently by neutron reflectometry and various other magnetic techniques, hydrogen absorption modifies the Fermi surface of the Nb layers which, in turn, changes the magnetic coupling and the associated magnetoresistivity effect in this system [Phys. Rev. Lett. **78** (1997) 1150].

THE SNS MAGNETISM REFLECTOMETER: BASIC DESIGN AND NEUTRON GUIDE OPTIMIZATION USING MONTE CARLO SIMULATIONS

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In this contribution, we summarize the optimization of the neutron guide optics of the Magnetism Reflectometer, which is currently under construction at the Spallation Neutron Source. The guide system consists of a straight source tube, a polygonal curved multi-channel bender, and a converging guide section. The bender will be essential for high-energy neutron and γ-ray background suppression, while the converging guide will focus the neutron beam onto the sample. Monte Carlo (MC) numerical methods were used to optimize the guide performance. –
The flux on sample and detector count rates were systematically determined for various guide configurations. The impact of guide imperfections like surface waviness and misalignment of sections are also studied.

THE INDIANA UNIVERSITY LOW ENERGY NEUTRON SOURCE

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We propose the construction of a long pulse cold neutron facility, using the existing infrastructure of the Indiana University Cyclotron facility. Neutrons will be produced from a direct proton to neutron reaction in lithium, stimulated by a pulsed 7 MeV proton beam. The neutrons will be moderated in a coupled solid methane moderator at 22 K; the neutron brightness at 4 meV is estimated to be the same or greater than that obtained at the IPNS on the H-moderator. Instruments for small angle scattering will be constructed, including a novel spin-echo SANS instrument, a conventional SANS instrument, and a radiography instrument. In all, structure covering 7 orders of magnitude in space will be observable with this suite. Science is proposed for these instruments covering hard and soft materials, biological samples, and moderator studies.

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